Modular magnetic field on the z-direction on a chain of nuclear spin system and quantum Not and Controlled-Not gates.

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February, 2010

Abstract

We study the simulation of a single qubit rotation and Controlled-Not gate in a solid state one-dimensional chain of nuclear spins system interacting weakly through an Ising type of interaction with a modular component of the magnetic field in the z-direction, characterized by $B_z(z,t) = Bo(z)\cos\delta t$. These qubits are subjected to electromagnetic pulses which determine the transition in the one or two qubits system. We use the fidelity parameter to determine the performance of the Not (N) gate and Controlled-Not (CNOT) gate as a function of the frequency parameter δ. We found that for $|\delta| \leq 10^{-3}\ MHz$, these gates still have good fidelity.

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1 Introduction

Almost any quantum system with at least two quantum levels may be used, in principle, for quantum computation. This one uses qubits (quantum bits) instead of bits to process information. A qubit is the superposition of any two levels of the system, called $|0\rangle$ and $|1\rangle$ states, $\Psi = C_0|0\rangle + C_1|1\rangle$ with $|C_0|^2 + |C_1|^2 = 1$. The tensorial product of L-qubits makes up a register of length L, say $|x\rangle = |i_{L-1}, ..., i_0\rangle$, with $i_j = 0, 1$, and a quantum computer with L-qubits works in a 2^L dimensional Hilbert space, where an element of this space is of the form $\Psi = \sum C_x|x\rangle$, with $\sum |C_x|^2 = 1$. Any operation with registers is done through a unitary transformation which defines a quantum gate, and one of the must important result about quantum gates and quantum logical operation is that any quantum computation can be done in terms of a single qubit unitary operation and a Controlled-Not (CNOT) gate Although quantum computers of few qubits [3]-[9] have been in to make serious computer calculations one may requires a quantum computer with at least of 100-qubits registers, and hopefully this will be achieved in a future not so far away. One solid state quantum computer model that has been explored for physical realization and which allows to make analytical and numerical studies of quantum gates and protocols [10] is the one made of one-dimensional chain of nuclear spins systems
[11]-[12] inside a strong magnetic field in the z-direction (with very strong gradient in that direction) and an RF-field in the transverse direction. Such a model physically is unlikely to be constructed, however this represents a good approximation for simulation of quantum algorithms and gates whose respective results could be applied in more realistic quantum computers. Furthermore, the approach relies in the universal character of Quantum Mechanics. In this model, the Ising interaction is considered among first and second neighbor spins which allows to implement ideally this type of computer up to 1000-qubits or more [13],[14]. Among other gates and algorithms [15], one qubit rotation and CNOT gates were study with this quantum computer model [16]. One of the important statement of this model is that one keep constant the magnetic field in the z-direction at the location of each qubit. However, this statement may be not so realistic in practice for this model or other solid state quantum computer based on spin system with very strong axial magnetic field, and then we wonder: if there is a magnetic field modulation where this field change slowly with time, how these basic elements, one qubit rotation and CNOT gates, would be Of course, in this case, the usual analytical approximation without field modulation is not valid anymore, and a full numerical calculation is required to see the possible effect of this modulation on 1-qubit rotations and CNOT gates.

In this paper, we want to study this modulation effect of the magnetic field on the Not (particular case of 1-qubit rotation, or unitary operation) and CNOT quantum gates. To do this, we will assume an additional cosine time dependence on the normal z-direction of the magnetic field and will determine, using the fidelity parameter, the minimum variation in the

frequency of this modulation to keep these quantum gates elements still well defined.

2 Quantum Not-gate

Consider a single paramagnetic particle with spin one-half in a magnetic field given by

$$\mathbf{B} = (B_a \cos(\omega t), -B_a \sin(\omega t), B_0(z) \cos \delta t) \tag{1}$$

where the first two components represent the RF-field, and the third component represents the strong magnetic field in this direction. The interaction between this particle and the magnetic field is given by the Hamiltonian $H = -\vec{\mu} \cdot \mathbf{B}$, where $\vec{\mu}$ is the magnetic moment of the particle which is related with the nuclear spin $\widehat{\mathbf{S}} = \hbar \widehat{\mathbf{I}}$ as $\vec{\mu} = \gamma \hbar \widehat{\mathbf{I}}$, with γ the gyromagnetic ratio of the particle. So, the Hamiltonian is

$$\widehat{H} = -\vec{\mu} \cdot \mathbf{B} = -\hbar \omega_o \cos \delta t \ \hat{I}_z - \frac{\hbar \Omega}{2}(\hat{I}_+ e^{i\omega t} + \hat{I}_- e^{-i\omega t}) \ , \tag{2}$$

where $\omega_o = \gamma B_0(z_o)$ (z_o is the location of the particle) is the Larmor frequency, $\Omega = \gamma B_a$ is the Rabi frequency, and $\hat{I}_\pm$ represents the ascent (descent) operator, $\hat{I}_\pm = \hat{I}_x \pm i\hat{I}_y$. If $|0\rangle$ and $|1\rangle$ are the two states of the spin one-half, one has that

$$\hat{I}_z|i\rangle = \frac{(-1)^i}{2}|i\rangle \ , \quad \hat{I}_+|0\rangle = |1\rangle \ , \quad \hat{I}_-|1\rangle = |0\rangle \ . \tag{3}$$

To solve the Schrödinger equation,

$$i\hbar \frac{\partial |\Psi\rangle}{\partial t} = \widehat{H}|\Psi\rangle \ , \tag{4}$$

one proposes a solution of the form

$$|\Psi\rangle = c_o(t)|0\rangle + c_1(t)|1\rangle \tag{5}$$

such that $|c_o|^2 + |c_1|^2 = 1$ at any time. Doing this, one gets the following ordinary differential equations

$$i\dot{c}_o = -\frac{\omega_o \cos \delta t}{2}c_o - \frac{\Omega}{2}c_1 e^{i\omega t} \tag{6a}$$

and

$$i\dot{c}_1 = +\frac{\omega_o \cos \delta t}{2}c_1 - \frac{\Omega}{2}c_o e^{-i\omega t} \ . \tag{6b}$$

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Choosing $c_0(t) = e^{i\omega t/2} d_0(t)$ and $c_1(t) = e^{-i\omega t/2} d_1(t)$ in above equations, one has

$$i\dot{d}_0 = +\frac{\omega - \omega_o \cos \delta t}{2} d_0 - \frac{\Omega}{2} d_1 \qquad (7a)$$

and

$$i\dot{d}_1 = -\frac{\omega - \omega_o \cos \delta t}{2} d_1 - \frac{\Omega}{2} d_0 \qquad (7b)$$

which, in turns, can be written as the following uncoupled similar Mathieu equation [19],

$$\ddot{d}_0 + \alpha(t) d_0 = 0 \qquad (8a)$$

where the complex function $\alpha(t)$ is given by

$$\alpha(t) = \frac{1}{4} \left[\Omega^2 + \omega^2 \left(1 - \frac{\omega_o}{\omega} \cos \delta t \right)^2 \right] + i \frac{\omega_o \delta}{2} \sin \delta t , \qquad (8b)$$

and d_1 is obtained from (7a),

$$d_1 = \frac{\omega - \omega_o \cos \delta t}{\Omega} d_0 - i \frac{2}{\Omega} \dot{d}_0 . \qquad (9)$$

For $\delta = 0$ and on resonance ($\omega = \omega_o$), one has that $\alpha = \Omega^2/4$, and the system oscillates between the states $|0\rangle$ and $|1\rangle$ with and angular frequency corresponding to the Rabi frequency Ω, as one expected [16]. For $\delta \neq 0$ the solution of this equation is far to be trivial, and instead of solving the Eq. (8a), we will find directly the numerical solution of the system (7) with the given initial conditions. By taking $\omega = \omega_o$ (resonant case), one expects to obtain the transition $|0\rangle \longleftrightarrow |1\rangle$ and to get the quantum Not-gate with a phase.

To study the performance of the quantum Not-gate as a function of the modulation frequency δ , we will calculate the fidelity parameter at the end of a π-pulse and make the comparison of the ideal wave function, $\Psi_{expected}$, with the wave function resulting from our simulation, Ψ_{sim}.

$$F = \langle \Psi_{sim} | \Psi_{expected} \rangle , \qquad (10)$$

where $|\Psi_{sim}\rangle$ is the state obtained from numerical simulations, and $|\Psi_{expected}\rangle$ is the ideal expected state. for the initial condition $|\Psi_o\rangle = |0\rangle$, of course, the fidelity coincide with the coefficient $|c_1|^2$. At this point we want to stress that we define $|F|^2$ in this way due that any quantum gate or algorithm is represented by the final wave function of the quantum system. Ideally, if the quantum gate is fully realizable this wave function is represented by $|\Psi_{expected}\rangle$. However, the non resonant transitions and the error systems (modulation) make that the resulting wave function of the complete simulation is given by $|\Psi_{sim}\rangle$. In this way, the fidelity is a measure of the good operation of gates and algorithms. On the other hand,

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there is another measurement for the calculation of the the distance between two states and this is the so called Uhlmann-Josza fidelity [17]. However, in Ref. [18] it has been shown that Eq. (10) is a lower bound for the Uhlmann-Josza fidelity. Such a result favors the present results.

Fig. 1a and Fig. 1b show the behavior of the fidelity and the probabilities as a function of the parameter δ at the end of a π-pulse, $\tau = \pi/\Omega$. We have used the parameters (units $2\pi \ MHz$) $\Omega = 0.1$ and $\omega_o = 200$. The RF-frequency has been chosen equal to the resonant frequency $\omega = \omega_o$. As one can see, for $\delta \leq 0.2 \times 10^{-3} MHz$ we can have a very well defined quantum Not-gate.

3 Two qubits model and quantum CNOT gate

Fig.2 shows two paramagnetic nuclear particles of spin one-half (qubits) subjected to a magnetic field of Eq. (1), making and angle $\cos\theta = \sqrt{3}/2$ to eliminate the dipole-dipole interaction between them. The interaction of the magnetic field with the qubits is carried out through the coupling with their dipole magnetic moment $\vec{\mu}_i = \gamma\mathbf{S}_i \ \ (i = 1, \ 2)$, where γ is the gyromagnetic ratio and $\widehat{\mathbf{S}}_i$ is the spin of the ith-nucleon ($\widehat{\mathbf{S}} = \hbar\widehat{\mathbf{I}}$). The interaction energy is given by

$$
\begin{aligned}
\widehat{H} &= -\vec{\mu}_1 \cdot \mathbf{B}_1 - \vec{\mu}_2 \cdot \mathbf{B}_2 + \hbar J \hat{I}_z^{(1)} \hat{I}_z^{(2)} \\
&= \widehat{H}_0 - \frac{\hbar\Omega}{2} \left(\hat{I}_+^{(1)} e^{i\omega t} + \hat{I}_-^{(1)} e^{-i\omega t} + \hat{I}_+^{(2)} e^{i\omega t} + \hat{I}_-^{(2)} e^{-i\omega t} \right),
\end{aligned} \tag{11}
$$

where J is the coupling constant of interaction between nearest neighboring spins, $\Omega = \gamma B_a$ is the Rabi frequency, $\widehat{H}_0$ is the part of Hamiltonian which is diagonal in the basis $\{|i_1 i_o\rangle\}_{i_j=0,1}$ and is given by

$$
\widehat{H}_0 = -\hbar \left(\omega_1 \hat{I}_z^{(1)} + \omega_2 \hat{I}_z^{(2)} \right) \cos\delta t + \hbar J \hat{I}_z^{(1)} \hat{I}_z^{(2)}. \tag{12}
$$

where ω_i are the Larmor's frequencies which are defined as

$$
\omega_i = \gamma B_0(z_i) \quad i = 1, 2 \tag{13}
$$

with z_i being the z-location of the ith-qubit. The eigenvalues of $\widehat{H}_0$ on the above basis for $\delta = 0$ are

$$
\begin{aligned}
E_{00} &= -\frac{1}{2}\{\omega_1 + \omega_2 - \frac{1}{2}J\} \quad E_{01} = -\frac{1}{2}\{\omega_1 - \omega_2 + \frac{1}{2}J\} \\
E_{10} &= -\frac{1}{2}\{-\omega_1 + \omega_2 + \frac{1}{2}J\} \quad E_{11} = -\frac{1}{2}\{-\omega_1 - \omega_2 - \frac{1}{2}J\}
\end{aligned} \tag{14}
$$

By doing $\omega = (E_{11} - E_{10})/\hbar = \omega_2 - J/2$, one gets the resonant transition which defines

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the CNOT operation $|10\rangle \longleftrightarrow |11\rangle$ with a phase involved $(e^{i\pi/2})$, where the left qubits is the control and the right one is the target. To solve the Schrödinger equation,

$$i\hbar\frac{\partial|\Psi\rangle}{\partial t} = \widehat{H}|\Psi\rangle \ ,\tag{15}$$

we can assume that the wave function can be written as

$$\Psi = C_{00}(t)|00\rangle + C_{01}(t)|01\rangle + C_{10}(t)|10\rangle + C_{11}(t)|11\rangle\tag{16}$$

such that $\sum|C_{ij}|^2 = 1$. Thus, we arrive to the following system of complex-couple ordinary differential equations

$$i\dot{C}_{00} = -\frac{1}{2}\left((\omega_1+\omega_2)\cos\delta t - \frac{1}{2}J\right)C_{00} - \frac{\Omega}{2}\left(C_{01}+C_{10}\right)e^{i\omega t}\tag{17a}$$

$$i\dot{C}_{01} = -\frac{1}{2}\left((\omega_1-\omega_2)\cos\delta t + \frac{1}{2}J\right)C_{01} - \frac{\Omega}{2}\left(C_{00}e^{-i\omega t} + C_{11}e^{i\omega t}\right)\tag{17b}$$

$$i\dot{C}_{10} = -\frac{1}{2}\left((\omega_2-\omega_1)\cos\delta t + \frac{1}{2}J\right)C_{10} - \frac{\Omega}{2}\left(C_{00}e^{-i\omega t} + C_{11}e^{i\omega t}\right)\tag{17c}$$

$$i\dot{C}_{11} = -\frac{1}{2}\left(-(\omega_1+\omega_2)\cos\delta t - \frac{1}{2}J\right)C_{11} - \frac{\Omega}{2}\left(C_{01}+C_{10}\right)e^{-i\omega t}.\tag{17d}$$

Doing the transformation $C_{00} = e^{i\omega t/2}D_{00}$, $C_{01} = e^{-i\omega t/2}D_{01}$, $C_{10} = e^{-i\omega t/2}D_{10}$, and $C_{11} = e^{-i3\omega t/2}D_{11}$, one gets rid of the fast oscillations and gets the following equations for the coefficients $D's$:

$$i\dot{D}_{00} = -\frac{1}{2}\left((\omega_1+\omega_2)\cos\delta t - \frac{1}{2}J - \omega\right)D_{00} - \frac{\Omega}{2}\left(D_{01}+D_{10}\right)\tag{18a}$$

$$i\dot{D}_{01} = -\frac{1}{2}\left((\omega_1-\omega_2)\cos\delta t + \frac{1}{2}J + \omega\right)D_{01} - \frac{\Omega}{2}\left(D_{00}+D_{11}\right)\tag{18b}$$

$$i\dot{D}_{10} = -\frac{1}{2}\left((\omega_2-\omega_1)\cos\delta t + \frac{1}{2}J + \omega\right)D_{10} - \frac{\Omega}{2}\left(D_{00}+D_{11}\right)\tag{18c}$$

$$i\dot{D}_{11} = -\frac{1}{2}\left(-(\omega_1+\omega_2)\cos\delta t - \frac{1}{2}J + 3\omega\right)D_{11} - \frac{\Omega}{2}\left(D_{01}+D_{10}\right).\tag{18d}$$

We solve numerically these equation, and for $\delta = 0$ and $\omega = \omega_2 - J/2$, a full transition will occur between the states $|10\rangle$ and $|11\rangle$. Note that one has $C_{ij}(0) = D_{ij}(0)$ and $|C_{ij}(t)|^2 = |D_{ij}(t)|^2$. For $\delta \neq 0$, we consider two initially conditions cases: Digital case, where the initial condition is given by

$$|\Psi_o\rangle = |10\rangle \ ,\tag{19a}$$

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that is $C_{00}(0) = 0$, $\quad C_{01}(0) = 0$, $\quad C_{10}(0) = 1$, $\quad C_{11}(0) = 0$. Superposition case, where the initial condition is

$$|\Psi_o\rangle = \sqrt{\frac{2}{10}}|00\rangle + \frac{1}{\sqrt{10}}|01\rangle + \sqrt{\frac{6}{10}}|10\rangle + \frac{1}{\sqrt{10}}|11\rangle \ . \tag{19b}$$

For our simulation, we use the following parameters (units $2\pi\ MHz$) $\Omega = 0.1$, $\omega_1 = 100$, $\omega_2 = 110$, and $J = 10$. The RF-frequency chosen is the resonant frequency $\omega = \omega_2 - J/2$, and applying a π-pulse, $\tau = \pi/\Omega$, we should get the respective CNOT transition $|10\rangle \longleftrightarrow |11\rangle$. Fig. 3 shows the behavior of the probabilities and the fidelity as a function of the parameter δ at the end of the π-pulse and for the digital case. Fig. 4 shows the same as before but for the superposition case. This case is more stable (the fidelity decays more slowly than the digital case) due to non zero contribution to the terms C_{00} and C_{01} which always contribute with the same constant probability $3/10$.

4   Conclusion

For a quantum computer model of a chain of qubits in a magnetic field where its z-component varies with respect the time, we have studied the Not and Controlled-Not gate behavior as a function of the frequency δ of variation of this component. In general, one can say that for $\delta \leq 10^{-3} MHz$ these quantum gates remain well defined with a fidelity very close to one. This small value in δ means that it is enough to consider a first order in taylor expansion of the cosine function in Eq. (1). We have seen that the fidelity for the superposition case is more stable than the digital case due to the contribution to the fidelity parameter of the other no zero states involved in the dynamics. Of course, this safety region, defined by δ, for these quantum gates does not mean safety for a full quantum algorithm, which is under studied.

5   Acknowledgments

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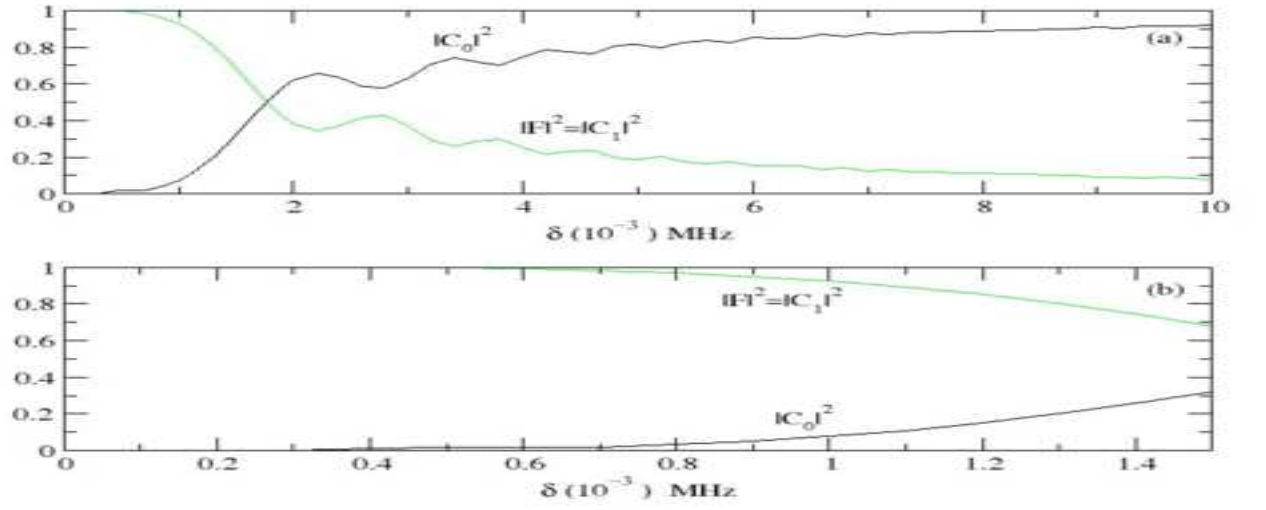
Figure 1: Quantum Not-gate: (a) Global behavior (b) Local behavior with respect to δ.
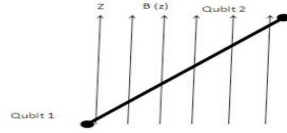
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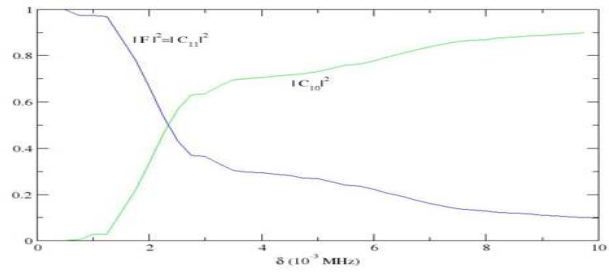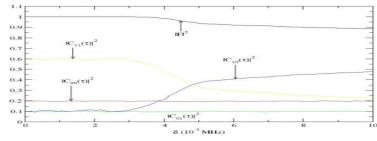Figure 2:   Two qubits configuration.

Figure 3:   CNOT behavior, digital case.

Figure 4: CNOT behavior, superposition case.